2-Nitrobenzamide

610-15-1 DTXSID002	5733

Model Performance

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	Model	I)ata
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Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 9.08e-09 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.77e-01

Confidence level: 3.45e-01

Nearest Neighbors from the Training Set

Image not found

3-Nitrotoluene

Measured: 1.20e-06 Predicted: 5.08e-02

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Profenofos

Measured: 6.45e-09 **Predicted:** 4.22e-06

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cis-Nonachlordane Measured: 1.20e-09 Predicted: 2.30e-06

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4-Nitrotoluene

Measured: 3.20e-06 Predicted: 3.88e-02